

Pairing in the Presence of a Pseudogap

T.A. Maier,¹ P. Staar,² and D.J. Scalapino³

¹Computer Science and Mathematics Division and Center for Nanophase Materials Sciences,
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6494, USA

²IBM Research – Zürich, CH-8803 Rüschlikon, Switzerland

³Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA

Evidence that the pseudogap (PG) in a near-optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ sample destroys the BCS logarithmic pairing instability [1] raises again the question of the role of the PG in the high-temperature superconducting cuprates [2]. The elimination of the BCS instability is consistent with the view that the PG competes with superconductivity. However, as noted in [1], the onset of superconductivity with a $T_c \sim 90$ K suggests an alternative scenario in which the PG reflects the formation of short range pairing correlations. Here, we report results obtained from a dynamic cluster quantum Monte Carlo approximation (DCA) for a 2D Hubbard model and conclude that (1) the PG, like the superconductivity, arises due to short-range antiferromagnetic correlations and (2) contrary to the usual case in which the pairing instability arises from the Cooper instability, here, the strength of the spin-fluctuations increases as the temperature decreases leading to the pairing instability.

The superconducting transition temperature can be determined from the Bethe-Salpeter gap equation

$$-\frac{T}{N} \sum_{n'k'} \Gamma_{\text{irr}}^{pp}(k, \omega_n, k', \omega_{n'}) G(k', \omega_{n'}) G(-k', -\omega_{n'}) \quad (1)$$

$$\times \phi_\alpha(k', \omega_{n'}) = \lambda_\alpha \phi_\alpha(k, \omega_n).$$

Here $G(k, \omega_n)$ is the dressed single particle Green's function, Γ_{irr}^{pp} the irreducible particle-particle pairing vertex and k and $\omega_n = (2n+1)\pi T$ are the usual momentum and Matsubara frequencies, respectively. The temperature at which the leading eigenvalue of Eq. (1) goes to 1 gives T_c and the corresponding eigenfunction $\phi_\alpha(k, \omega_n)$ determines the symmetry of the gap. In spin fluctuation theories the pairing vertex is approximated by an effective interaction

$$V_{\text{eff}}(q, \omega_m) = \frac{3}{2} \bar{U}^2 \chi(q, \omega_m) \quad (2)$$

with $\chi(q, \omega_m)$ the spin susceptibility and \bar{U} a coupling strength. Various groups have used experimental data to model $\chi(q, \omega_m)$, $G(k, \omega_n)$ and \bar{U} in order to determine whether a spin-fluctuation pairing interaction is consistent with the observed T_c values.

Dahm et al. [3] used inelastic neutron scattering (INS) measurements for $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ to model the spin susceptibility $\chi(q, \omega_m)$ and a one-loop self-energy approximation to determine G . \bar{U} was an adjustable parameter estimated from INS and ARPES data. Using the resulting G and V_{eff} in Eq. (1), they concluded that a spin-fluctuation interaction had sufficient strength to account for the observed T_c . Nishiyama *et al.* [4] used inelastic neutron scattering results for $\chi(q, \omega)$ and solved the Eliashberg equations for the heavy fermion compounds CeCuSi_2 and CeIrIn_3 . For reasonable values of \bar{U} , they found T_c values which were again consistent with the notion that antiferromagnetic spin fluctuations were responsible for pairing in these materials. In a recent paper Mishra, *et al.* [1] used angular resolved photoemission spectroscopy (ARPES) data for a slightly underdoped BSCCO ($T_c = 90\text{K}$) sample to examine the effect of the pseudogap (PG) on the superconducting transition temperature and to determine whether a spin-fluctuation pairing mechanism could account for the observed T_c . They found that the usual BCS logarithmic divergence associated with the propagators in Eq. (1) was destroyed by the pseudogap and the leading eigenvalue $\lambda_d(T)$ remained small, and was essentially independent of temperature. This raises old questions regarding the interplay between the PG and superconductivity [2] which continue to be of interest [5–8]. Here, using the dynamic cluster approximation (DCA), we explore spin-fluctuation pairing in a Hubbard model which exhibits a PG.

The two-dimensional Hubbard model we will consider has a near neighbor hopping t , a next near neighbor hopping $t'/t = -0.15$, an onsite Coulomb interaction $U/t = 7$ and a filling $\langle n \rangle = 0.92$. We will work in energy units where $t = 1$. The DCA calculations [9] were carried out on a 4×4 cluster and employed both continuous-time, auxiliary-field (CT-AUX) quantum Monte Carlo (QMC) [10] and Hirsch-Fye (HF) QMC [11] methods to solve the effective cluster problem [12]. In the DCA approximation, where Γ_{irr}^{pp} depends only on a finite set of cluster momenta K , the k -sum in Eq. (1) gives [13]

$$-\frac{T}{N_c} \sum_{n', K'} \Gamma_{\text{irr}}^{pp}(K, \omega_n, K', \omega_{n'}) \bar{\chi}_0^{pp}(K', \omega_{n'}) \phi_\alpha(K', \omega_{n'}) \quad (3)$$

$$= \lambda_\alpha \phi_\alpha(K, \omega_n).$$

Here $N_c = 16$ is the cluster size and the pairing kernel

$G(k, \omega_n)G(-k, -\omega_n)$ has been coarse-grained (averaged) over the momenta k' of the DCA patches

$$\bar{\chi}_0^{pp}(K, \omega_n) = \frac{N_c}{N} \sum_{k'} G(K + k', \omega_n) G(-K - k', -\omega_n). \quad (4)$$

For the parameters we have chosen, the uniform static susceptibility $\chi(q = 0, T)$ versus temperature, shown in Fig. 1a, exhibits a peak at $T^* = 0.22$ below which

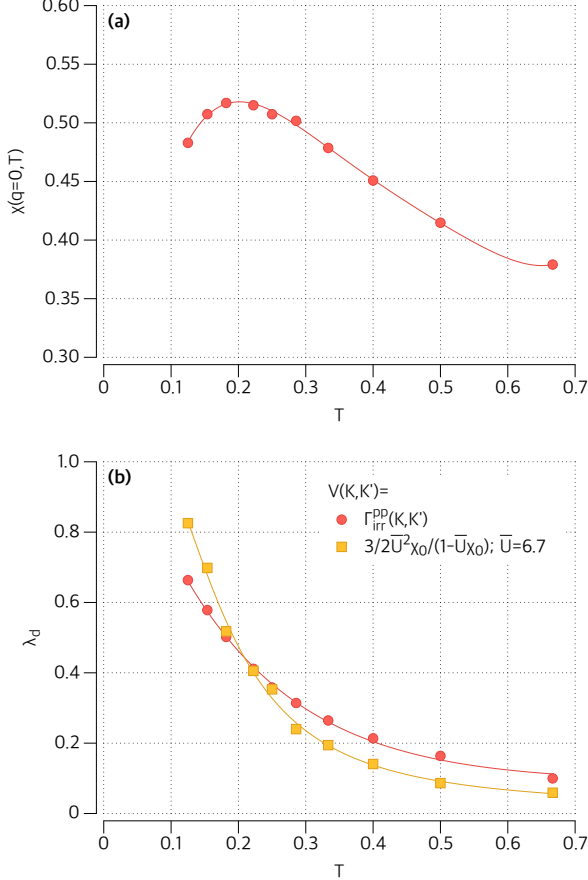


FIG. 1. **Pairing in the presence of a pseudogap.** (a) The uniform static spin susceptibility $\chi(q = 0, T)$ versus temperature for $\langle n \rangle = 0.92$ $t' = -0.15$ and $U = 7$ peaks at a temperature $T^* = 0.22$ and decreases below this as the pseudogap opens. (b) The leading eigenvalue $\lambda_d(T)$ of the particle-particle Bethe-Salpeter equation versus temperature (circles) from a DCA calculation of Γ_{irr}^{pp} . The d -wave eigenvalue for the spin-fluctuation interaction with $\chi(q, \omega_m)$ the RPA spin susceptibility from Eq. 8 and $\bar{U} = 6.7$ is shown as the solid squares.

it decreases as T is reduced [14]. This behavior, seen in measurements of the magnetic susceptibility [15] and Knight shifts [16] of underdoped (hole) cuprates, reflects the opening of a pseudogap. ARPES experiments [17, 18] find that this gap is anisotropic, opening in the antinodal regions of the Fermi surface. This behavior has also been

seen in DCA calculations of the single-particle spectral weight [14, 19]. In Fig. 1b, the temperature dependence of the leading eigenvalue of the Bethe-Salpeter equation (3) is shown as the circles. Its eigenfunction has d -wave symmetry and $\lambda_d(T)$ approaches 1 at low temperatures. Thus this model system has a pseudogap that opens below T^* and a d -wave eigenvalue that increases towards 1 as T decreases.

In addition to suppressing the $q = 0$ spin susceptibility, we find that the opening of the pseudogap destroys the low temperature BCS logarithmic divergence of the d -wave projection of the pairing kernel

$$P_{0d}(T) = -\frac{T}{N_c} \sum_{K, \omega_n} \phi_d(K, \omega_n) \bar{\chi}_0^{pp}(K, \omega_n) \phi_d(K, \omega_n) \quad (5)$$

Here, $\bar{\chi}_0^{pp}(K, \omega_n)$ is defined in Eq. (4) and $\phi_d(k, \omega_n)$ is the d -wave eigenfunction, which is approximated as

$$\phi_d(k, \omega_n) \sim \begin{cases} (\cos k_x - \cos k_y) & |\omega_n| < J \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

with $J \sim 4t^2/U$. A plot of $P_{0d}(T)$ versus T is shown in Fig. 2a and one can see that below T^* , $P_{0d}(T)$ is suppressed as the pseudogap opens [20, 21]. Here we have normalized $P_{0d}(T)$ to its value at a temperature $T = 0.5t$ above T^* . For comparison, the solid squares in Fig. 2a show $P_{0d}(T)$ for $\langle n \rangle = 0.85$ which does not have a pseudogap and one sees the usual BCS logarithmic behavior (dashed curve).

The absence of the BCS divergence in $P_{0d}(T)$ when there is a pseudogap is consistent with the finding of Mishra *et al.* [22]. However, as noted, they found that with this suppression, the spin-fluctuation pairing interaction failed to give a superconducting transition. Based on this, they suggested that the pseudogap reflects the presence of short-range pairfield correlations which grow below T^* and become coherent at T_c . This behavior could be likened to the magnetic response of the large U half-filled Hubbard model. In this case, the formation of local moments when the temperature drops below $\sim U/2$ is seen in an increase in the expectation value of the square of the local moment $\langle S_z^2 \rangle = \langle (\frac{1}{2}(n_\uparrow - n_\downarrow))^2 \rangle$. In a similar way one can look for the onset of local pair formation as T decreases below the pseudogap temperature T^* . Here with $\Delta_{\ell+x, \ell}^\dagger = c_{\ell+x \uparrow}^\dagger c_{\ell \downarrow}^\dagger - c_{\ell+x \downarrow}^\dagger c_{\ell \uparrow}^\dagger$ and $\Delta_d^\dagger = (\Delta_{\ell+x, \ell}^\dagger - \Delta_{\ell+y, \ell}^\dagger + \Delta_{\ell-x, \ell}^\dagger - \Delta_{\ell-y, \ell}^\dagger)$, we have calculated $\langle \Delta_d^\dagger \Delta_d \rangle$ versus temperature. As shown in Fig. 2b, this correlation function does increase as the temperature decreases. However, the four near neighbor pairfield correlations

$$\langle \Delta_{\ell+x, \ell}^\dagger \Delta_{\ell+x, \ell} \rangle = \frac{1}{2} \langle n_\ell n_{\ell+x} \rangle - 6 \langle S_\ell^z S_{\ell+x}^z \rangle, \quad (7)$$

contribute the dominant contribution to this increase as shown in Fig. 2b. These results suggest that the pseudogap is more closely related to the formation of short range

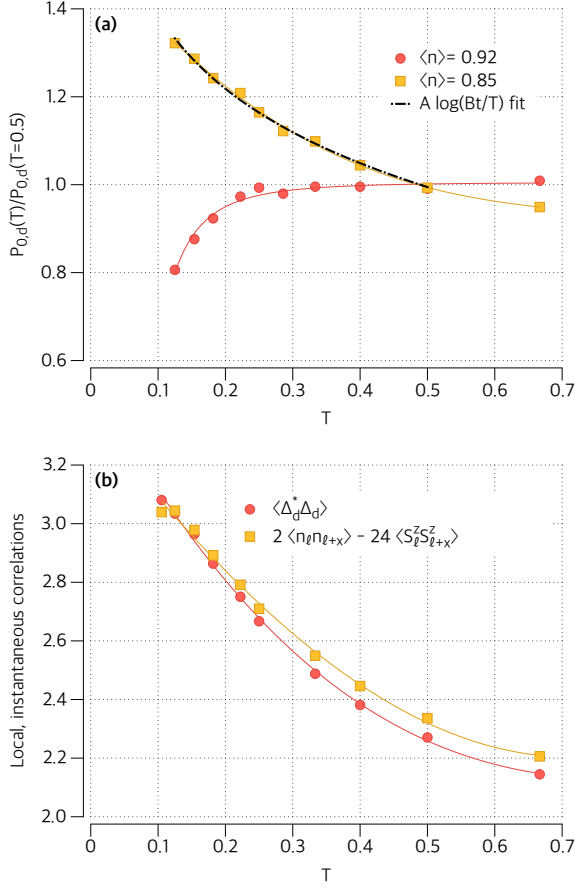


FIG. 2. **Destructure of the BCS logarithmic instability and nature of local pairing correlations.** (a) The logarithmic BCS increase of the d -wave projection of the pairing kernel $P_{0d}(T)$ for $\langle n \rangle = 0.92$ is suppressed by the opening of the pseudogap (circles). Here $P_{0d}(T)$ has been normalized to 1 at a temperature $T = 0.5t$ above T^* . At temperatures below T^* , where the pseudogap has opened, the BCS logarithmic divergence is suppressed. The solid squares show $P_{0d}(T)$ for a filling $\langle n \rangle = 0.85$ where there is no pseudogap and one sees the usual logarithmic increase as the temperature decreases. (b) The temperature dependence of the local d -wave pairfield correlation function $\langle \Delta_d^+ \Delta_d \rangle$ (circles). The observed increase in $\langle \Delta_d^+ \Delta_d \rangle$ as T decreases below T^* reflects the development of near neighbor AF correlations (squares).

antiferromagnetic correlations than to local pair correlations in agreement with earlier ideas of Johnston [15] and more recent theoretical results [5–8, 23]. This identification of the PG with the development of short-range AF spin correlations is also consistent with the increase of the spin-susceptibility $\chi(Q = (\pi, \pi), \omega_m = 0)$ as shown in Fig. 3 and as seen experimentally [24].

Returning to the question of whether the spin-fluctuation interaction, Eq. (2), can lead to superconductivity when the logarithmic singularity of the BCS kernel is suppressed, we use DCA results for $G(k, \omega_n)$ to construct $V_{\text{eff}}(q, \omega_m)$. Here, following Mishra *et al.*, an

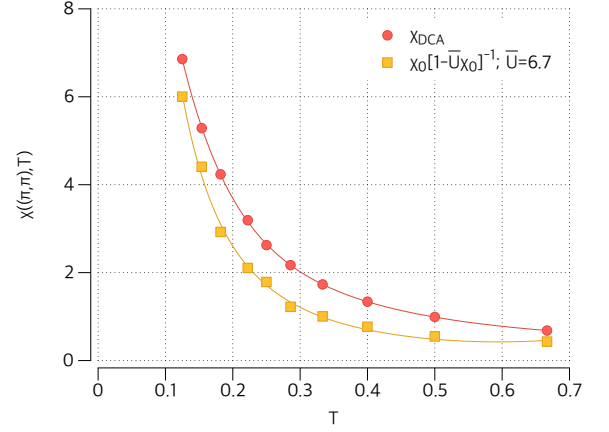


FIG. 3. **DCA spin susceptibility and RPA fit.** The AF spin susceptibility $\chi_{\text{DCA}}(Q = (\pi, \pi), \omega_m = 0)$ from the DCA calculation (circles) and the RPA fit, Eq. (8), with $\bar{U} = 6.7$ (squares). The AF response continues to increase as T decreases below T^* leading to an increase of the spin-fluctuation interaction so that even though the BCS logarithmic increase of $P_0(T)$ is suppressed, the d -wave eigenvalue $\lambda_d(T)$ increases as seen in Fig. 2.

RPA form for χ is used

$$\chi_{\text{RPA}}(Q, \omega_m) = \frac{\chi_0(Q, \omega_m)}{1 - \bar{U}\chi_0(Q, \omega_m)} \quad (8)$$

with

$$\chi_0(Q, \omega_m) = \frac{T}{N_c} \sum_K \bar{G}(K + Q, \omega_n + \omega_m) \bar{G}(K, \omega_n), \quad (9)$$

where $\bar{G}(K, \omega_n) = N_c/N \sum_{k'} G(K + k', \omega_n)$ is the DCA coarse-grained Green's function. The coupling \bar{U} is estimated from the approximate fit of χ_{RPA} to χ_{DCA} shown in Fig. 3.

Then, replacing Γ_{irr}^{pp} by V_{eff} and using DCA Green's functions, we solve the Bethe-Salpeter equation (3). Results for $\lambda_d(T)$ are shown (solid squares) in Fig. 2. We conclude that the increase in the strength of the pairing interaction V_{eff} leads to an increasing $\lambda_d(T)$ similar to that which is found using Γ_{irr}^{pp} determined from the DCA calculation. Thus, in spite of the absence of the BCS logarithmic increase in $P_{0d}(T)$, we find that the increase in the strength of the spin-fluctuations leads to an increase in $\lambda_d(T)$ as the temperature is lowered. This differs from the results of reference [1] and we speculate that this difference arises from a failure of their parametrization of $G(k, \omega_n)$ by ARPES data taken at 140 K as the temperature is lowered.

To summarize, we have used DCA calculations for an under (hole) doped 2D Hubbard model, which exhibits a pseudogap, to see whether a spin-fluctuation interaction provides a reasonable approximation of the irreducible pairing interaction. In this calculation, the dynamic

mean-field cluster is such that charge density and striping instabilities are suppressed, leaving antiferromagnetic and d -wave pairing as the dominant correlations. We find that while the pseudogap eliminates the usual BCS logarithmic divergence of the pairing kernel, a pairing instability arises from an increase in the strength of the spin-fluctuation interaction as the temperature decreases.

ACKNOWLEDGMENTS

The authors want to thank V. Mishra and M.R. Norman for useful discussions and for sending them a plot of $P_{0d}(T)$ calculated using their ARPES derived single particle Greens function. The authors also want to thank E. Gull, S. R. Kivelson, A.-M. Tremblay, and L. Taillefer for useful comments. DJS and TAM acknowledge the support of the Center for Nanophase Materials Science at ORNL, which is sponsored by the Division of Scientific User Facilities, U.S. DOE. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

-
- [1] Vivek Mishra, U. Chatterjee, J. C. Campuzano, and M. R. Norman, *Nat. Phys.* **10**, 357 (2014).
 - [2] M. R. Norman, D. Pines, C. Kallin, *Adv. Phys.* **54**, 715 (2005).
 - [3] T. Dahm *et al.*, *Nat. Phys.* **5**, 217 (2009).
 - [4] S. Nishiyama, K. Miyake and C.M. Varma, *Phys. Rev. B* **88**, 014510 (2013).
 - [5] G. Sordi, P. Sémon, K. Haule, A.-M. S. Tremblay, *Phys. Rev. Lett.* **108**, 216401 (2012).
 - [6] Kuang-Shing Chen, Zi Yang Meng, Shu-Xiang Yang, Thomas Pruschke, Juana Moreno, Mark Jarrell, *Phys. Rev. B* **88**, 245110 (2013).
 - [7] O. Gunnarsson, T. Schäfer, J.P.F. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer, A. Toschi, arXiv:1411.6947.
 - [8] E. Gull, O. Parcollet, A. J. Millis, *Phys. Rev. Lett.* **110**, 216405 (2013).
 - [9] Th. Maier, M. Jarrell, Th. Pruschke, M.H. Hettler, *Rev. Mod. Phys.* **77**, 1027 (2005).
 - [10] E. Gull, P. Werner, O. Parcollet, M. Troyer, *Europhys. Lett.* **82**, 57003 (2008).
 - [11] J. Hirsch, R. Fye, *Phys. Rev. Lett.* **56**, 2521 (1986).
 - [12] The data in Figs. 1, 2a and 3 was obtained with CT-AUX QMC and cross-checked with HF QMC. The equal-time data in Fig. 2b was obtained with HF QMC.
 - [13] T. A. Maier, M. Jarrell, D. Scalapino, *Phys. Rev. B* **74**, 094513 (2006).
 - [14] C. Huscroft, M. Jarrell, Th. Maier, S. Moukouri, and A. N. Tahvildarzadeh, *Phys. Rev. Lett.*, **86**, 139 (2001).
 - [15] David C. Johnston, *Phys. Rev. Lett.* **62**, 957 (1989).
 - [16] H. Alloul, T. Ohno, and P. Mendels, *Phys. Rev. Lett.* **3**, 1700 (1989).
 - [17] D. S. Marshall, D. S. Dessau, A. G. Loeser, C. H. Park, A. V. Matsuura, J. N. Eckstein, I. Bozovic, P. Fournier, A. Kapitulnik, W.E. Spicer and Z.-X. Shen, *Phys. Rev. Lett.* **76**, 4841 (1996).
 - [18] M.R. Norman, H. Ding, M. Randeria, J.C. Campuzano, T. Yokoya, T. Takouchi, T. Takahashi, T. Mochiku, K. Kadowaki, P. Guptasarma, and D. G. Hinks, *Nature* **392**, 157 (1998).
 - [19] E. Gull, M. Ferrero, O. Parcollet, A. Georges, A. Millis, *Phys. Rev. B* **82**, 155101 (2010).
 - [20] B. Kyung, J.-S. Landry, and A.-M. S. Tremblay, *Phys. Rev. B* **68**, 174502 (2003).
 - [21] S.-X. Yang *et al.*, *Phys. Rev. Lett.* **106**, 047004 (2011).
 - [22] $P_{0d}(T)$ is the d -wave projection of what Mishra *et al.* [1] referred to as the pairing kernel.
 - [23] T. Sakai and Y. Takahashi, *J. Phys. Soc. Jpn.* **70**, 272 (2001).
 - [24] S. Ouazi, J. Bobroff, H. Alloul and W.A. MacFarlane, *Phys. Rev. B* **70**, 104515 (2004).